Supplemental material

Xenobiotica

Intestinal phase-II metabolism of quercetin in HT29 cells, 3D human intestinal tissues and in healthy volunteers: a qualitative comparison using LC-IMS-MS and LC-HRMS

Figure S1. CCS calibration plot for poly-DL-alanine (n = 3–12) with nitrogen as a drift gas in negative ionization mode. Corrected drift time (t_D') corresponds to mass-independent drift time. Normalized CCS (Ω') corresponds to CCS values (in Å^2) times the square root of the reduced mass divided by charge state. More detailed explanations can be found in the Supporting information of (Paglia *et al.*, 2014)

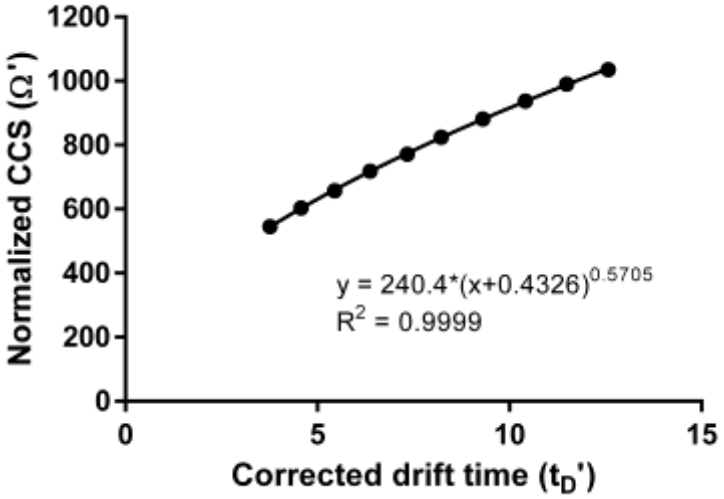
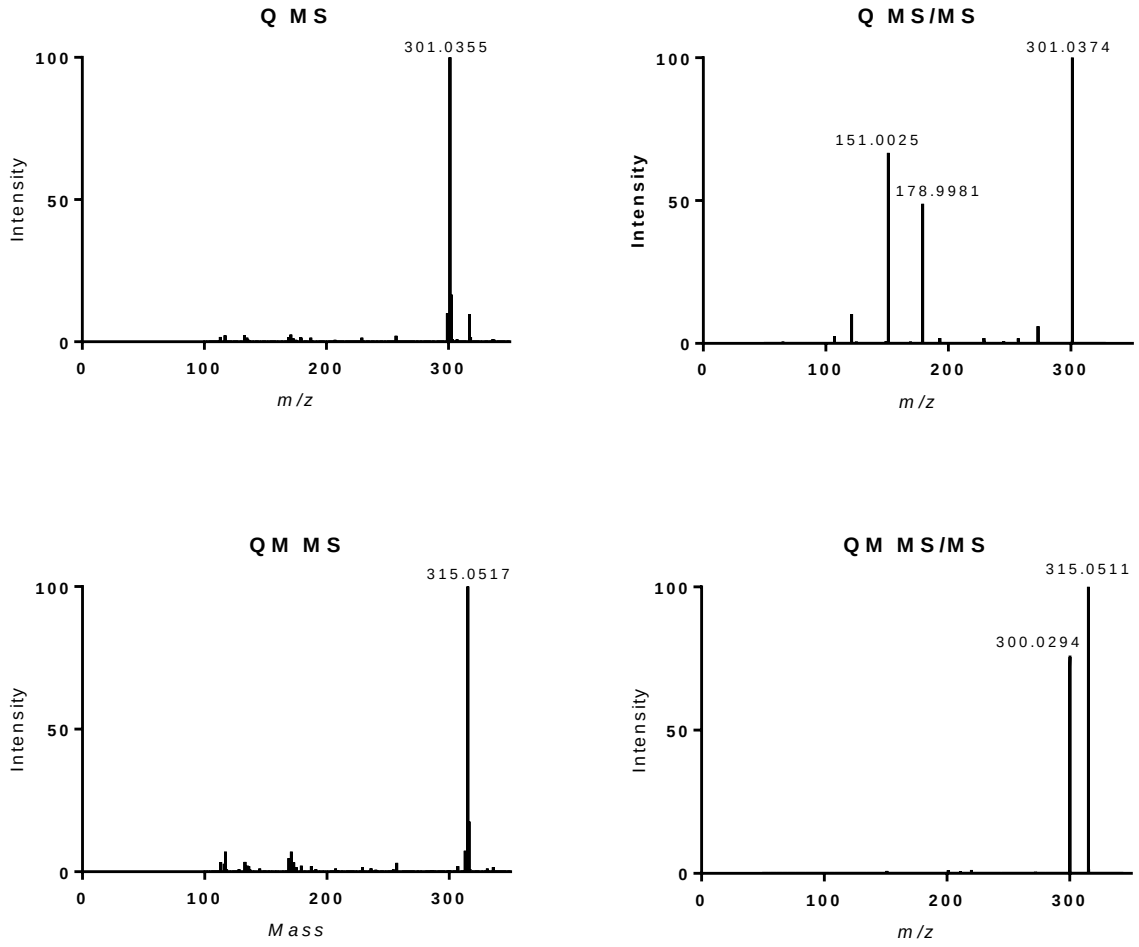
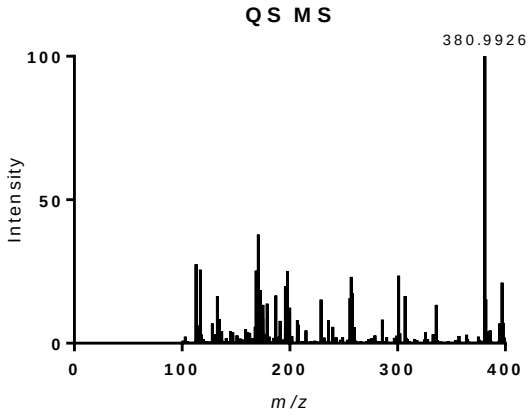
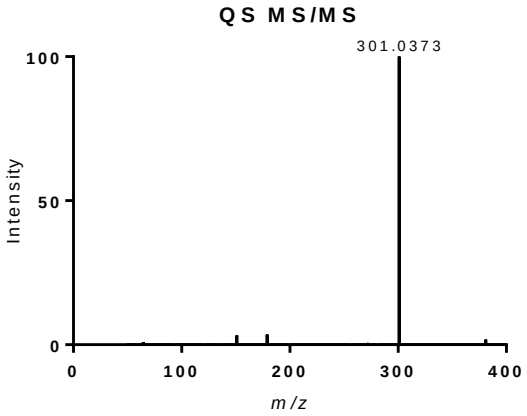
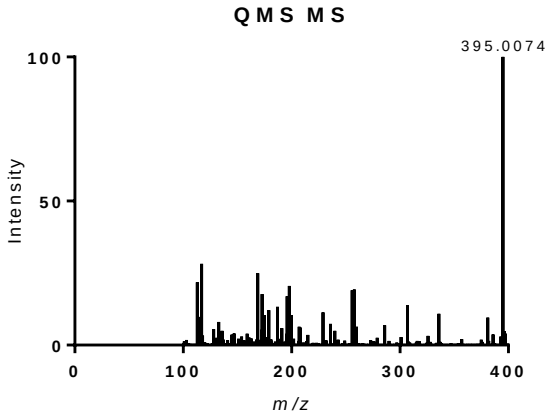


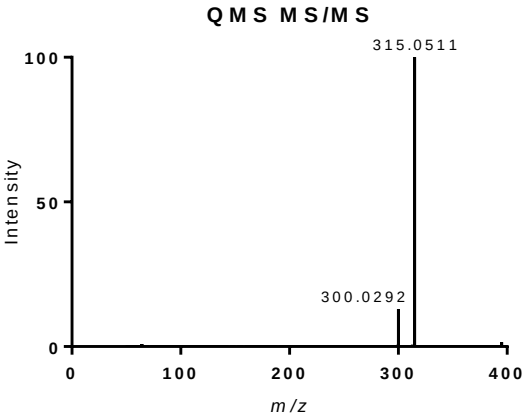
Figure S2. MS and dd-MS^2 (data-dependent MS^2) spectra of quercetin (Q), methylquercetin (QM), quercetin sulfate (QS), methylquercetin sulfate (QMS), quercetin glucuronide (QG) and methylquercetin glucuronide (QMG)

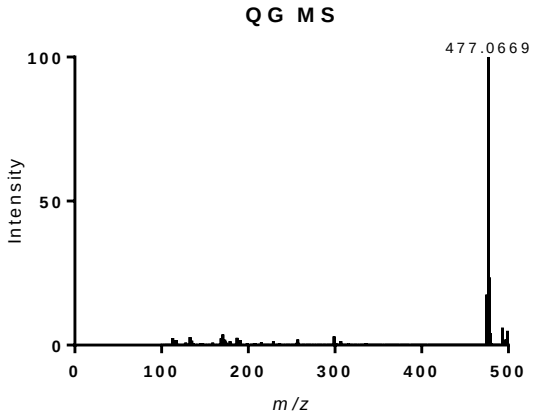


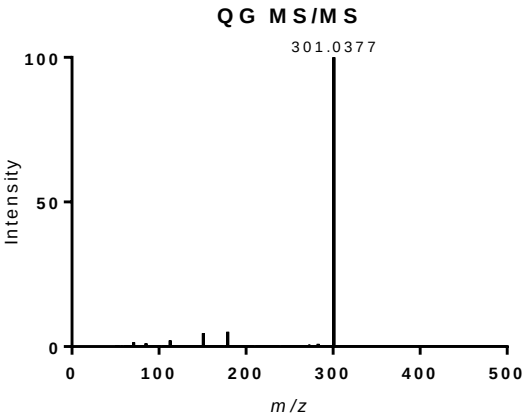

QS MS
380.9926
Intensity
m/z

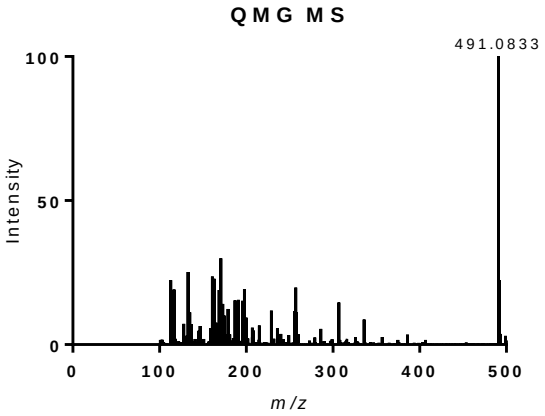

QS MS/MS
301.0373
Intensity
m/z


QMS MS
395.0074
Intensity
m/z


QMS MS/MS
315.0511
300.0292
Intensity
m/z


QG MS
477.0669
Intensity
m/z


QG MS/MS
301.0377
Intensity
m/z


QMG MS
491.0833
100
50
0
Intensity
0
100
200
300
400
500
m/z

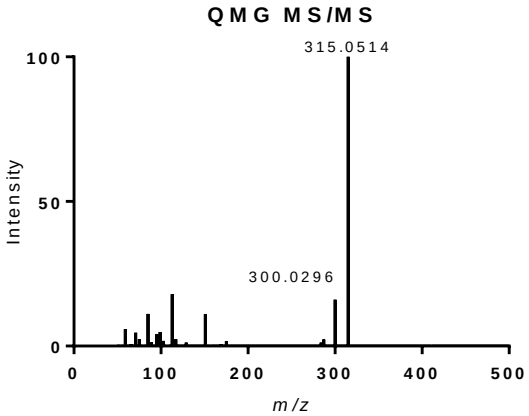

QMG MS/MS
315.0514
300.0296
100
50
0
Intensity
0
100
200
300
400
500
m/z

Table S1. Calculated CCS values of the quercetin glucuronides (QGs) obtained with the Avogadro software (v. 1.1.1) and the CCS calculation tool of DriftScope (v. 2.1). The full description of the procedure can be found in full in (Chalet *et al.*, 2018).

Molecule	Calculated CCS ($Å^2$)	Experimental CCS ($Å^2$)
Q3G	181	200
Q4'G	191	209
Q3'G	187	195
Q7G	188	205
Q5G	193	210

References

Chalet, C., Hollebrands, B., Janssen, H.G., Augustijns, P. & Duchateau, G., 2018. Identification of phase-II metabolites of flavonoids by liquid chromatography-ion-mobility spectrometry-mass spectrometry. *Anal Bioanal Chem,* 410**,** 471-482.

Paglia, G., Williams, J.P., Menikarachchi, L., Thompson, J.W., Tyldesley-Worster, R., Halldorsson, S., Rolfsson, O., Moseley, A., Grant, D., Langridge, J., Palsson, B.O. & Astarita, G., 2014. Ion mobility derived collision cross sections to support metabolomics applications. *Anal Chem,* 86**,** 3985-3993.